

Computer Program Abstracts

The category Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Following normal submission, a Computer Program Abstract will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 of the June 1985 issue of the Journal [*J. Appl. Cryst.* (1985), **18**, 189–190].

J. Appl. Cryst. (1991). **24**, 1079

FRDICT – *ab initio* generation of FRODO dictionary. By M. V. HOSUR, *Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Bombay - 4000 85, India.*

(Received 20 June 1991;
accepted 25 June 1991)

The crystallographic problem: Crystallographic and modelling methods can form the basis for rational design of new molecules (Bugg & Ealick, 1990). The interactive computer graphics programs *FRODO/TOM/O* (Jones, 1978; Jones, Bergdoll & Kjeldgaard, 1990) are being extensively used to provide the necessary structural information on proteins and protein-inhibitor complexes. An important feature of these programs is their REFI option, in which molecular fragments distorted while fitting into electron density or while achieving desired interactions with other molecules are ultimately refined to proper stereochemistry defined in a dictionary. This dictionary is an ordered atom list of the molecule, along with a list matrix whose structure has been described by Hermans & Ferro (1971). We have described previously (Prasad & Hosur, 1991) a procedure and a computer program, *FRDICT*, to generate automatically a *FRODO* dictionary for any new group, given Cartesian coordinates of the group. In a molecular design experiment the structural formula of the molecule itself is a variable parameter and atomic coordinates may not be available (Gund, Andose, Rhodes & Smith, 1980). An extension of the *FRDICT* program (Prasad & Hosur, 1991) to accept molecular input through specification of only the structural formula is reported here. Thus *FRDICT* now operates in two modes: (a) *ab initio* mode (present report) and (b) coordinate mode.

Method of solution: The structural formula is input through two files, FILE1 and FILE2, whose actual names are read from the terminal (see below).

For a molecular group of N atoms, FILE1 is an $N \times N$ matrix ((MAT(I,J), $I = 1, N$), $J = 1, N$) of integer elements. MAT(I,J) is zero if there is no covalent bond between atoms I and J.

$$\text{MAT}(I,J) = \begin{cases} 1 & \text{if bond (I,J) is a} \\ & \text{single bond} \\ 2 & \text{if bond (I,J) is a} \\ & \text{double bond} \end{cases}$$

FILE2 is a single-record file of N integer variables. A value of 1 or 2 for the i th variable denotes sp^3 or sp^2 hybridization respectively for the i th atom in the input. In addition to these files, the following information is read through the terminal interactively: (a) a four-character alphanumeric name for the group; (b) number of atoms N and whether the structural formula is input (Yes or No); (c) name of the data file containing atom names and coordinates (one atom per record); (d) name of the data file giving atom connectivities (FILE1); (e) name of the data file giving hybridization type of atoms (FILE2). Records (d) and (e) are not asked for if the answer to the second part of (b) is No. In this case the atom-names file should also contain coordinates of each atom and *FRDICT* runs in the coordinate mode.

Using the connectivity information given in MAT(I,J), the atomic ordering for the dictionary is done as described previously (Prasad & Hosur, 1991). The program then scans this ordered atom list and fills the columns of the list matrix relating to stereochemical information. Each atom is given a code number based on the first character of its name and its hybridization and these numbers are used to pick out from a stored data base appropriate standard bond lengths (Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987). In making this choice the program also uses the bond types input through the structural formula of the group. In the case of ring structures *FRDICT* generates dictionaries for planar rings in its *ab initio* mode of operation. The program automatically finds the number of atoms in the ring and sets the endocyclic and exocyclic angles to appropriate values. To generate a *FRODO* dictionary for a puckered ring, the easiest route would be to run *FRDICT* twice, first in the *ab initio* mode to generate the planar ring, modify this ring interactively to produce the required pucker, output the coordinates using the SAM option of *FRODO* and then rerun *FRDICT* a second time on these coordinates. The proper stereochemistry at an asymmetric carbon atom is ensured by appropriate ordering in the input stream of atoms bonded to the asymmetric carbon atom.

Software and hardware environments, program specification availability: The program, 700 lines long, is written in standard Fortran77 and does not use either overlay structure or any special library programs. The dictionary produced by *FRDICT* has been successfully used with *FRODO/TOM* installed on Silicon Graphics IRIS 3100 and IRIS 4D/20 workstations. Copies of the program can be obtained from the author.

Keywords: molecular design, dictionary, *FRODO*, protein.

I sincerely thank Professor M. A. Viswamitra, Dr K. K. Kannan and S. C. Chakravarty for many stimulating discussions. I am also grateful to the BARC Computer Centre staff for their help.

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
- Bugg, C. E. & Ealick, S. E. (1990). Editors. *Crystallographic and Modeling Methods in Molecular Design*. New York: Springer Verlag.
- Gund, P., Andose, J. D., Rhodes, J. B. & Smith, G. M. (1980). *Science*, **208**, 1425–1431.
- Hermans, J. Jr & Ferro, D. (1971). *Biopolymers*, **10**, 1121–1138.
- Jones, T. A. (1978). *J. Appl. Cryst.* **11**, 268–272.
- Jones, T. A., Bergdoll, M. & Kjeldgaard, M. (1990). In *Crystallographic and Modeling Methods in Molecular Design*, edited by C. E. Bugg & S. E. Ealick, pp. 189–200. New York: Springer Verlag.
- Prasad, V. & Hosur, M. V. (1991). *J. Appl. Cryst.* **24**, 405–406.

Meeting Report

J. Appl. Cryst. (1991). **24**, 1079–1080

The First European Powder Diffraction Conference (EPDIC 1), München, Germany, 14–16 March 1991

The First European Powder Diffraction Conference was held at the Institute of Natural Sciences of Ludwig-Maximilian University in Munich. The Conference was also sponsored by the International Union of Crystallography, JCPDS–International Centre for Diffraction Data

and Arbeitsgemeinschaft für Kristallographie. Dr H. E. Göbel was the Organizing Committee Chairman and Dr J. Visser was the Programme Committee Chairman. Approximately 220 participants from 24 countries took part in the activities. During the meeting a commercial exhibition was organized, showing recent developments in hardware and software in the field of X-ray studies. More than twenty companies, including Siemens, Philips, Seifert, Enraf-Nonius, Stoe and Nicolet, took part. Demonstrations and a workshop concerning the JCPDS-ICDD powder diffraction file and other crystallographic databases were perfectly prepared.

The two and a half days scientific programme was opened by an honorary lecture by Professor H. Jagodzinski on 'The Role of Munich for X-ray Powder Crystallography and the History of X-ray Powder Diffraction'. It was followed by 16 main lectures dedicated to areas of general interest: 'X-ray Diffraction Profiles Due to Real Polycrystals' by P. Klimanek, 'Quo Vadis Quantitative Powder Diffraction Analysis' by J. Fiala, 'Crystal Structure Analysis and Refinement by the Two-Step Method' by G. Will, 'Neutron Powder Diffraction and Oxide Superconductors' by A. W. Hewat, 'Applied Crystallography in Advanced Ceramics' by R. L. Snyder, 'New Instrumentation in Powder Diffraction' by J. Ihringer, 'New Detectors in X-ray Diffraction' by P. Tucker, 'Energy Dispersive XRPD at High Pressure' by L. Gerward, 'Glory and Misery of the Structure Analysis of Thin Polycrystalline Films' by V. Valvoda, 'Characterization of Epitaxial Thin Films by X-ray Diffraction' by A. Segmüller, 'Powder Diffraction Using Synchrotron Radiation' by M. Hart, 'X-ray Absorption and Reflection in Materials Science' by B. Lengeler, 'Preferred Orientation in Powder Diffraction' by H.-J. Bunge, 'X-ray Stress Analysis' by J. M. Sprael, 'On the Use of Rietveld Refinements for Structural Studies' by P.-E. Werner, 'Indexing of Powder Diffraction Patterns' by D. Louër. 54 other oral contributions and 120 posters were also presented.

It is difficult to mention all the lectures which were of the greatest interest, but some of them have to be pointed out. Among these, a contribution by A. W. Hewat describing one of the most exciting applications of high-resolution neutron diffraction ever performed, the HRTEM photos presented by H. Budin showing the sinusoidal orientation of unit cells in the Bi-based superconductors and a talk given by J. Schneider demonstrating even anharmonic temperature factor

analysis which can be carried out in combination with the X-ray and neutron Rietveld method. Real structure was one of the main fields of the conference. Lectures on texture by H.-J. Bunge, inhomogeneity by P. Klimanek and V. Valvoda were also the center of interest. Surface roughness was discussed in some papers (N. Masciocchi, B. Lengeler). B. Greenberg described the new QPD system developed in Philips Laboratories designed in connection with real structure problems.

The high level of the meeting should be maintained during EPDIC 2, which will take place on the campus of the University of Twente, the Netherlands, from 30 July to 1 August 1992.

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ECC Chairman

Crystallographers

J. Appl. Cryst. (1991), **24**, 1080–1081

This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

F. L. Hirshfeld 1927–1991

Fred Hirshfeld arrived at the Weizmann Institute in 1951 armed with a Master's degree in mathematics from Columbia, a sharp mind and a deep faith in the precepts of Torah Judaism. All these were to remain with him until his untimely passing, from the ravages of a rapidly developing cancer, in May 1991. Coupled to these intellectual assets were some very human qualities – an ability to tolerate and accept people whose views on many subjects were very different from his own, and a willingness to help others that ranged from the critical review of manuscripts *in statu nascendi* to knuckling down to details of organizing meetings, summer schools and committees.

Hirshfeld soon showed his mettle in Rehovoth. His abilities as a constructive critic led Gerhard Schmidt to include him as a co-author on Schmidt's first paper on intramolecular overcrowding [*J. Chem. Soc.* (1954), pp. 3288–3294], even though he had made no experimental contribution to the work described – but his participation was an essential factor in the development and description of the then-novel ideas. Moreover, despite his theoretical bent and background, Hirshfeld became an active experimentalist in Schmidt's early exploitation of the advantages of liquid-

N₂ low temperatures in crystal structure analysis [*J. Chem. Phys.* (1957), **26**, 923–929].

Hirshfeld really found his metier in the field of electron density studies. Here he was a pioneer, as shown by a long series of careful studies involving both experimental measurements and theoretical analyses. The term 'deformation density' dates from this period. One of Hirshfeld's last papers was a review (*Electron Density Distributions in Molecules*) in *Crystallogr. Rev.* [(1991), **2**, 169–201] which he was able to see just before he died. This was an area, with its combination of the need for careful definition of objectives, accurate and exacting experimental measurement and deep theoretical analysis, which admirably suited Hirshfeld's personality.

Despite his concentration on electron density studies, other characteristic, and still quoted, papers appeared from time to time in the crystallographic literature. An early and noteworthy contribution was his definition of the Cheshire groups [*Acta Cryst.* (1968), **A24**, 301–311], the groups of minimal symmetry needed for determining possible molecular arrangements from a real-space comparison of observed and calculated structure factors. The elegance of this work was typical of Hirshfeld's approach, even if its current practical importance has been diminished by our present plethora of computing power. This was followed by discussion, together with Dov Rabinovich [*Acta Cryst.* (1973), **A29**, 510–513], of whether reflections with intensities measured as negative should be included in least-squares analyses. Another relates to the relative vibration amplitudes of pairs of atoms along the vector joining them. Hirshfeld's criterion [*Acta Cryst.* (1976), **A32**, 239–244] that this value should be less than 10 pm² in a rigid molecule is often applied as a test of intramolecular rigidity, while deviation from this norm gives information about internal vibrations and disorder.

Hirshfeld was an active participant in the life of the crystallographic community. He was Chairman of the Israel Crystallographic Society in 1973, an organizer of the Bat-Sheva Seminar on Electron Density Mapping in Molecules and Crystals held in Rehovoth in 1977 and Editor of the Report (*Isr. J. Chem.* (1977), **16**, 87–231], a member of the Editorial Board of *Isr. J. Chem.* for a number of years in the 1970's, a member of the Organizing Committee of ECM-7 (Jerusalem, 1982) (and displayed hitherto unknown talents as graphics designer of the Book of Abstracts), a member of the Commission on Crystallographic Data of the